ABSTRACT

The present invention relates generally to biotechnology and information technology, and in particular, to a subfield known as bioinformatics. A specific aspect of the invention lies in the provision of a new method and system for predicting the three-dimensional structure of proteins. The main focus in this patent application is on the

5   development of a globally optimal and practically efficient threading algorithm based on an alignment model incorporating pairwise interaction preferences explicitly, and allowing variable gaps by using an integer programming approach. Integer programming formulation can fully exploit the abovementioned special features of the pairwise interaction preferences. It allows one to use the existing powerful linear

10   programming packages together with a branch and bound algorithm to rapidly arrive at the optimal alignment. This is the first time that integer programming and linear programming has been applied to protein threading.